Dopants, non-stoichiometry and defects versus topologically non-trivial surface electronic states in Bi_2Se_3 and Bi_2Te_3

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Abstract

Although topological insulators (TI) such as single-crystalline Bi_2Se_3 and Bi_2Te_3 possess unique properties of metallic surface states having a Dirac cone structure, which pave the way for advanced technologies, their practical applications are still limited. One of the factors that restrict their practical use is the insufficient control over the details of the electronic structure details, such as the position of the Fermi level relative to the electronic states of the surface and volume. This leads to unwanted bulk conductivity, which dominates the surface properties of TIs.

The thesis proposes several methods for manipulating the electronic structure of TIs in order to improve their characteristics. The impact of these methods on a range of parameters was investigated using high-sensitivity surface characterization techniques such as scanning tunneling microscopy and spectroscopy (STM/STS), angle-resolved photoelectron spectroscopy (ARPES), low-energy electron diffraction (LEED), and Auger electron spectroscopy (AES). The experimental measurements were compared to calculations based on density functional theory (DFT). The studies were complemented by magnetotransport measurements at temperatures below 1 K, allowing for observations of Shubnikov–de Haas quantum oscillations.

Studies on Bi_2Se_3 doped with Mg and Fe atoms have shown that both dopants modify the surface states with Dirac cone structure, affecting parameters such as the radius of Fermi surface and effective mass of carriers. It has been demonstrated that doping with Fe atoms causes a significant shift of the Fermi level deep into the volume conduction band. Interestingly, the topological states on the surface were found to be resistant to the introduction of these dopants. In particular, on the magnetic dopant of Fe, as magnetic dopants may tend to destroy the non-trivial topology of the system.

Deviations from the perfect stoichiometry of Bi_2Te_3 has been found to have a significant impact on the conductivity character of the material and the distribution of structural defects. A series of samples synthesized as a function of Te concentration conditions show a change from p-type conductivity for the stoichiometric compound to n-type conductivity for clearly over-stoichiometric Te concentrations. The most important result obtained is the demonstration that the change in conductivity character occurs through a smooth shift of the Fermi level position as a function of Te concentration, from the volume valence band to the gap for the volume states and finally to the volume conduction band. It was also shown that surface states with linear dispersion are present in all samples within the investigated range of Te concentrations. This means that there are Te concentrations at which the Fermi level can be located in the gap for volume states where only topologically protected surface states exist.

One of the results obtained in the study is the dependence of the properties of the surface electronic states on the statistical distribution of defects in the crystal lattice of Bi_2Te_3. Thermal treatment of Bi_2Te_3 was used as a method to excite the diffusion of structural defects in the material, which can lead to significant changes in the statistics of their distribution in the sample, such as agglomeration in near-surface layers. The mentioned diffusion was directly observed in the measurements, but it was found that it does not ultimately lead to drastic changes in the defect statistics near the surface, nor therefore in the electronic structure. Upon reaching a certain temperature, the formation of a new phase was observed, covering fractions of the surface of Bi_2Te_3 with a locally different electronic structure than the surface of the initial material, even after annealing. The global nature of the conductivity of the sample, whose large surface areas are covered by the new phase, remains undisturbed. Furthermore, it was confirmed that topological surface states are resistant to partial coverage of the surface with another phase and are present in annealed samples in areas where the atomic configuration has not changed.

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